Karin Fink

List of Publications by Year in descending order

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90 papers	3,470 citations	147801 31 h-index	149698 56 g-index
97 all docs	97 docs citations	97 times ranked	5693 citing authors

#	Article	IF	Citations
1	Zinc Oxide Nanoparticles with Defects. Advanced Functional Materials, 2005, 15, 1945-1954.	14.9	499
2	Active Sites on Oxide Surfaces: ZnO-Catalyzed Synthesis of Methanol from CO and H2. Angewandte Chemie - International Edition, 2005, 44, 2790-2794.	13.8	192
3	Electrical control over the Fe(II) spin crossover in a single molecule: Theory and experiment. Physical Review B, 2011, 83, .	3.2	169
4	Stabilization of Polar ZnO Surfaces: Validating Microscopic Models by Using CO as a Probe Molecule. Physical Review Letters, 2003, 90, 106102.	7.8	164
5	Switching of a coupled spin pair in a single-molecule junction. Nature Nanotechnology, 2013, 8, 575-579.	31.5	107
6	Interfacial dominated ferromagnetism in nanograined ZnO: a Î¼SR and DFT study. Scientific Reports, 2015, 5, 8871.	3.3	97
7	Ab Initio Calculation of the Magnetic Exchange Coupling in Linear Oxo-Bridged Binuclear Complexes of Titanium(III), Vanadium(III), and Chromium(III). Inorganic Chemistry, 1994, 33, 6219-6229.	4.0	89
8	Expanding the Coordination Cage: A Ruthenium(II)â^'Polypyridine Complex Exhibiting High Quantum Yields under Ambient Conditions. Inorganic Chemistry, 2009, 48, 5677-5684.	4.0	73
9	Field-Induced Slow Magnetic Relaxation in the Ni(I) Complexes [NiCl(PPh₃)₂]Â·C₄H₈O and [Ni(N(SiMe₃)₂)(PPh₃)₂]. Inorganic Chemistry, 2016, 55, 2091-2100.	4.0	73
10	Magnesium Anode for Chloride Ion Batteries. ACS Applied Materials & Interfaces, 2014, 6, 10997-11000.	8.0	69
11	Toward Onâ€andâ€Off Magnetism: Reversible Electrochemistry to Control Magnetic Phase Transitions in Spinel Ferrites. Advanced Functional Materials, 2016, 26, 7507-7515.	14.9	69
12	The Surface Science Approach for Understanding Reactions on Oxide Powders: The Importance of IR Spectroscopy. Angewandte Chemie - International Edition, 2012, 51, 4731-4734.	13.8	68
13	Defects as Color Centers: The Apparent Color of Metalâ€“Organic Frameworks Containing Cu²⁺-Based Paddle-Wheel Units. ACS Applied Materials & Interfaces, 2017, 9, 37463-37467.	8.0	60
14	Superexchange and Spinâ^'Orbit Coupling in Chlorine-Bridged Binuclear Cobalt(II) Complexes. Inorganic Chemistry, 1999, 38, 3847-3856.	4.0	59
15	[2.2]Paracyclophane derived bisphosphines for the activation of hydrogen by FLPs: application in domino hydrosilylation/hydrogenation of enones. Dalton Transactions, 2012, 41, 9056.	3.3	58
16	Experimental and theoretical investigations of the electronic band structure of metal-organic frameworks of HKUST-1 type. Applied Physics Letters, 2015, 107, .	3.3	57
17	Magnetic anisotropy of a Co^{II} single ion magnet with distorted trigonal prismatic coordination: theory and experiment. Physical Chemistry Chemical Physics, 2016, 18, 30135-30143.	2.8	56
18	A quantum chemical ab initio study of the superexchange coupling in binuclear oxygen-bridged Ni(II) complexes. Chemical Physics, 1995, 192, 25-35.	1.9	50

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19	Exploiting Synergies in Catalysis and Gas Sensing using Noble Metalâ€Loaded Oxide Composites. ChemCatChem, 2018, 10, 864-880.	3.7	50
20	The Formal Combination of Three Singlet Biradicaloid Entities to a Singlet Hexaradicaloid Metalloid Ge₁₄[Si(SiMe₃)₃]₅[Li(THF)₂]₃ Cluster. Journal of the American Chemical Society, 2011, 133, 2518-2524.	13.7	49
21	Ab Initio Study of the Adsorption of Small Molecules on Metalâ€“Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. Inorganic Chemistry, 2015, 54, 8251-8263.	4.0	48
22	Ab initio cluster calculations on the electronic structure of oxygen vacancies at the polar ZnO(0001Ì„) surface and on the adsorption of H2, CO, and CO2 at these sites. Physical Chemistry Chemical Physics, 2006, 8, 1482.	2.8	46
23	Catalytic subsurface etching of nanoscale channels in graphite. Nature Communications, 2013, 4, 1379.	12.8	46
24	Carbon incorporation effects and reaction mechanism of FeOCl cathode materials for chloride ion batteries. Scientific Reports, 2016, 6, 19448.	3.3	43
25	Divergent Coordination Chemistry: Parallel Synthesis of [2Ã—2] Iron(II) Gridâ€Complex Tautoâ€Conformers. Angewandte Chemie - International Edition, 2016, 55, 10881-10885.	13.8	41
26	Selective Coordination Bonding in Metalloâ€Supramolecular Systems on Surfaces. Angewandte Chemie - International Edition, 2012, 51, 4327-4331.	13.8	40
27	An ab initio study of the geometry dependence of the magnetic exchange coupling in oxo-bridged binuclear chromium(III) complexes. Chemical Physics, 1995, 201, 87-94.	1.9	39
28	Interaction of carboxylic acids with rutile TiO2(110): IR-investigations of terephthalic and benzoic acid adsorbed on a single crystal substrate. Surface Science, 2016, 643, 117-123.	1.9	39
29	Metal Complexes of a Redoxâ€Active [1]Phosphaferrocenophane: Structures, Electrochemistry and Redoxâ€Induced Catalysis. Chemistry - A European Journal, 2017, 23, 7402-7408.	3.3	35
30	Field-Induced Co(II) Single-Ion Magnets with mer-Directing Ligands but Ambiguous Coordination Geometry. Inorganic Chemistry, 2017, 56, 6056-6066.	4.0	35
31	Uniform Ï€â€System Alignment in Thin Films of Templateâ€Grown Dicarbonitrileâ€Oligophenyls. Advanced Functional Materials, 2011, 21, 1631-1642.	14.9	32
32	The Interaction of Formic Acid with Zinc Oxide: A Combined Experimental and Theoretical Study on Single Crystal and Powder Samples. Topics in Catalysis, 2015, 58, 174-183.	2.8	32
33	Ab initio cluster calculations for the absorption energies of F and F+ centers in bulk ZnO. Physical Chemistry Chemical Physics, 2005, 7, 2999.	2.8	31
34	Size and Isotope Effects of Helium Clusters and Droplets: Identification of Surface and Bulk-Volume Excitations. Journal of Physical Chemistry A, 2011, 115, 7316-7326.	2.5	31
35	NMR-Spectroscopic and Solid-State Investigations of Cometal-Free Asymmetric Conjugate Addition: A Dinuclear Paracyclophaneimine Zinc Methyl Complex. Journal of the American Chemical Society, 2010, 132, 12899-12905.	13.7	29
36	Homoleptic 1-D iron selenolate complexesâ€”synthesis, structure, magnetic and thermal behaviour of 1âˆž[Fe(SeR)2] (R = Ph, Mes). Dalton Transactions, 2011, 40, 7022.	3.3	29

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37	Spin-Crossover and Massive Anisotropy Switching of 5d Transition Metal Atoms on Graphene Nanoflakes. Nano Letters, 2014, 14, 3364-3368.	9.1	28
38	An ab initio cluster study of the magnetic properties of the CoO(001) surface. Chemical Physics, 2002, 278, 79-87.	1.9	27
39	Magnetic Properties of Paddlewheels and Trinuclear Clusters with Exposed Metal Sites. ChemPhysChem, 2011, 12, 3307-3319.	2.1	27
40	Interkingdom Signaling: Integration, Conformation, and Orientation of N-Acyl-<scp>l</scp>-homoserine Lactones in Supported Lipid Bilayers. Langmuir, 2012, 28, 8456-8462.	3.5	27
41	Abinitiocalculations of van der Waals interactions in oneâ€•and twoâ€dimensional infinite periodic systems. Journal of Chemical Physics, 1995, 103, 2603-2614.	3.0	26
42	Bi- and trimetallic rare-earthâ€“palladium complexes ligated by phosphinoamides. Chemical Communications, 2015, 51, 11761-11764.	4.1	26
43	Experimental characterization and simulation of amino acid and peptide interactions with inorganic materials. Engineering in Life Sciences, 2018, 18, 84-100.	3.6	26
44	Lithium-promoted hydrogenation of carbon dioxide to formates by heterobimetallic hydridozinc alkoxideclusters. Chemical Communications, 2008, , 73-75.	4.1	25
45	The method of local increments for the calculation of adsorption energies of atoms and small molecules on solid surfaces : Part I. A single Cu atom on the polar surfaces of ZnO. Physical Chemistry Chemical Physics, 2009, 11, 11196.	2.8	25
46	Binding patterns of homo-peptides on bare magnetic nanoparticles: insights into environmental dependence. Scientific Reports, 2017, 7, 14047.	3.3	25
47	An ab initio study of the adsorption of CO on a Zn4O4 cluster with wurtzite-like structure. Chemical Physics, 2003, 287, 183-195.	1.9	24
48	Ab initio study of the magnetic exchange coupling constants of a structural model [CaMn3IIIMnII] of the oxygen evolving center in photosystem II. Physical Chemistry Chemical Physics, 2009, 11, 3900.	2.8	23
49	Ab initio calculation of the magnetic exchange coupling in linear oxo-bridged heterobinuclear complexes of titanium (III), vanadium (III), and chromium (III). International Journal of Quantum Chemistry, 2000, 76, 137-147.	2.0	21
50	Charge Density Analysis of 2-Methyl-4-nitro-1-phenyl-1H-imidazole-5-carbonitrile: An Experimental and Theoretical Study of Câ‰¡NÂ·Â·Â·Câ‰¡N Interactions. Journal of Physical Chemistry A, 2011, 115, 12941-12952.	2.5	21
51	Ab initio cluster calculations of the magnetic properties of ZnO doped with transition metal ions. Chemical Physics, 2006, 326, 297-307.	1.9	20
52	Synthesis and Structure of an â€œIron-Dopedâ€•Copper Selenide Cluster Molecule: [Cu₃₀Fe₂Se₆(SePh)₂₄(dppm)₄]. Inorganic Chemistry, 2009, 48, 8977-8984.	4.0	19
53	Tris(3,5â€dimethylpyrazolyl)methaneâ€Based Heterobimetallic Complexes that Contain Znï£¿ and Cdï£¿Transitionâ€Metal Bonds: Synthesis, Structures, and Quantum Chemical Calculations. Chemistry - A European Journal, 2015, 21, 2905-2914.	3.3	19
54	Q and Soret Band Photoexcitation of Isolated Palladium Porphyrin Tetraanions Leads to Delayed Emission of Nonthermal Electrons over Microsecond Time Scales. Journal of Physical Chemistry Letters, 2016, 7, 1167-1172.	4.6	19

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55	Band-gap engineering with a twist: Formation of intercalant superlattices in twisted graphene bilayers. Physical Review B, 2015, 91, .	3.2	18
56	[Sn₄Si{Si(SiMe₃)₃}₄{SiMe₃}₂]: A Model Compound for the Unexpected Firstâ€Order Transition from a Singlet Biradicaloid to a Classical Bonded Molecule. Angewandte Chemie - International Edition, 2011, 50, 7273-7277.	13.8	17
57	A modified CAS-CI approach for an efficient calculation of magnetic exchange coupling constants. Molecular Physics, 2013, 111, 2594-2605.	1.7	15
58	Synthesis, Electronic Structure, and Structural Characterization of the New, â€œNon-Innocentâ€• 4,5-Dithio-Catecholate Ligand, Its Metal Complexes, and Their Oxidized 4,5-Dithio-o-quinone Derivatives. Inorganic Chemistry, 2009, 48, 8830-8844.	4.0	14
59	Deuterium-labelled N-acyl-l-homoserine lactones (AHLs)â€”inter-kingdom signalling moleculesâ€”synthesis, structural studies, and interactions with model lipid membranes. Analytical and Bioanalytical Chemistry, 2012, 403, 473-482.	3.7	14
60	Enantiopure Benzamidinate/Cyclooctatetraene Complexes of the Rare-Earth Elements: Synthesis, Structure, and Magnetism. Organometallics, 2018, 37, 3708-3717.	2.3	14
61	The spin coupling in the diiron complex [Fe2(hpdta)(H2O)3Cl]. Physical Chemistry Chemical Physics, 2007, 9, 1911-1920.	2.8	13
62	Adsorption of single Cu atoms at differently stabilized polar ZnO surfaces: An ab initio study. Journal of Computational Chemistry, 2008, 29, 2302-2310.	3.3	13
63	Cu(II)- and Mn(III)-Porphyrin-Derived Oligomeric Multianions: Structures and Photoelectron Spectra. Journal of Physical Chemistry A, 2014, 118, 369-379.	2.5	13
64	Effects of hydrogen ion irradiation on zinc oxide etching. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2017, 35, .	2.1	13
65	Mononuclear and dinuclear heteroleptic Cu(I) complexes based on pyridyl-triazole and DPEPhos with long-lived excited-state lifetimes. Journal of Organometallic Chemistry, 2018, 871, 140-149.	1.8	13
66	Tuning the Coordination Geometry and Magnetic Relaxation of Co(II) Single-Ion Magnets by Varying the Ligand Substitutions. Crystal Growth and Design, 2021, 21, 1035-1044.	3.0	13
67	A quantum chemical approach towards the electronically excited states of helium clusters. European Physical Journal D, 2007, 43, 121-124.	1.3	12
68	Formation and desorption of nickel hexafluoroacetylacetonate Ni(hfac)2 on a nickel oxide surface in atomic layer etching processes. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, .	2.1	12
69	Heteroâ€bimetallic Lanthanideâ€Coinage Metal Compounds Featuring Possible Metalâ€Metal Interactions in the Excited State. Chemistry - A European Journal, 2021, 27, 15128-15136.	3.3	12
70	How molecular oxygen binds to bis[trifluoroacetylacetonato(â^'1)]cobalt(ii) â€“ab initio and density functional theory studies. Dalton Transactions, 2011, 40, 11289.	3.3	10
71	Theoretical Approach Towards the Understanding of Asymmetric Additions of Dialkylzinc to Enals and Iminals Catalysed by [2.2]Paracyclophaneâ€Based N,Oâ€Ligands. Chemistry - A European Journal, 2012, 18, 8377-8385.	3.3	10
72	Development and Application of a Complete Active Space Spinâ€Orbit Configuration Interaction Program Designed for Single Molecule Magnets. ChemPhysChem, 2022, 23, .	2.1	10

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73	A fascinating multifaceted redox-active chelating ligand: introducing the N,Nâ€²-dimethyl-3,3â€²-biquinoxalinium â€œmethylbiquinoxenâ€•platform. Chemical Science, 2016, 7, 3820-3828.	7.4	8
74	Photodissociation of Free Metalloporphyrin Dimer Multianions. Journal of Physical Chemistry A, 2018, 122, 2974-2982.	2.5	8
75	Gas-Phase Ion Chemistry of Metalloporphyrin Anions with Molecular Oxygen: Probing the Influence of the Oxidation and Spin State of the Central Transition Metal by Experiment and Theory. Journal of Physical Chemistry A, 2018, 122, 4357-4365.	2.5	8
76	Enhanced etching of tin-doped indium oxide due to surface modification by hydrogen ion injection. Japanese Journal of Applied Physics, 2018, 57, 06JC05.	1.5	8
77	Autoionization spectroscopy of CO on metal oxide surfaces. Journal of Electron Spectroscopy and Related Phenomena, 1996, 77, 155-171.	1.7	7
78	Comment on â€œExcitations in photoactive molecules from quantum Monte Carloâ€•[J. Chem. Phys. 121, 5836 (2004)]. Journal of Chemical Physics, 2005, 122, 087101.	3.0	6
79	Trinuclear Early/Lateâ€Transitionâ€Metal Thiolate Complexes. European Journal of Inorganic Chemistry, 2014, 2014, 3510-3520.	2.0	6
80	Terminal Ligand and Packing Effects on Slow Relaxation in an Isostructural Set of [Dy(H₂dapp)X₂]⁺ Single Molecule Magnets**. Chemistry - A European Journal, 2021, 27, 15086-15095.	3.3	6
81	Rational Design of Iron Oxide Binding Peptide Tags. Langmuir, 2019, 35, 8472-8481.	3.5	5
82	Ab initiocalculation of potential energy surfaces for the three lowest triplet states (1â€‰3Aâ€²â€²,1â€‰3A,2â€‰3Aâ€²â€²) of PH(X,A)â€“He. Journal of Chemical Physics, 1997, 106, 7637-7641.	3.0	4
83	Magnetic anisotropy of graphene quantum dots decorated with a ruthenium adatom. Beilstein Journal of Nanotechnology, 2013, 4, 441-445.	2.8	4
84	Combining wavefunction frozen-density embedding with one-dimensional periodicity. Journal of Chemical Physics, 2021, 154, 104114.	3.0	4
85	Densityâ€functional study on the migration of Cd and Te adsorbates on the (001) surface of CdTe. Physica Status Solidi (B): Basic Research, 2010, 247, 937-944.	1.5	3
86	The Adsorption of Small Molecules on the Copper Paddle-Wheel: Influence of the Multi-Reference Ground State. Molecules, 2022, 27, 912.	3.8	2
87	Asymmetrically Difunctionalized 1,1â€²â€Ferrocenyl Metalloligands and Their Transition Metal Complexes. European Journal of Inorganic Chemistry, 2022, 2022, .	2.0	1
88	Ab initio Cluster Calculations for the Absorption Energies of F and F+ Centers in Bulk ZnO.. ChemInform, 2005, 36, no.	0.0	0
89	Ab initio calculations on the magnetic properties of transition metal complexes. AIP Conference Proceedings, 2015, , .	0.4	0
90	Frontispiece: Terminal Ligand and Packing Effects on Slow Relaxation in an Isostructural Set of [Dy(H₂dapp)X₂]⁺ Single Molecule Magnets. Chemistry - A European Journal, 2021, 27, .	3.3	0